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THE MASTER PROGRAM FILE, METHODS AND MODELS.(U)
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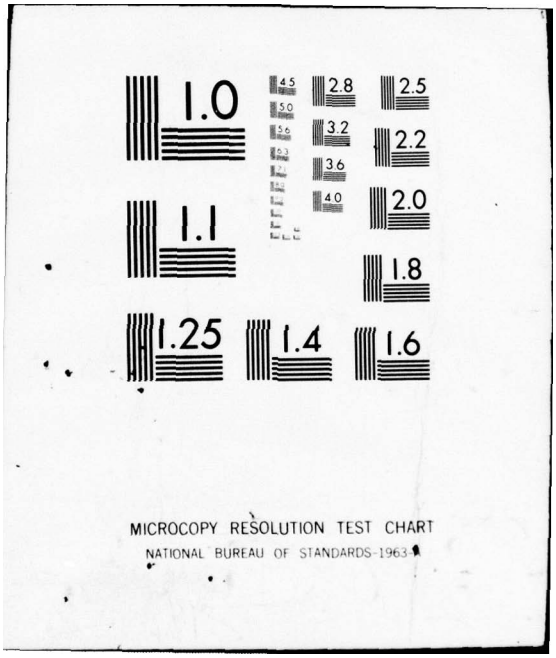
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THE MASTER PROGRAM FILE, METHODS AND MODELS

Experimental & Mathematical Physics
Santa Monica, CA 90403

May 1977

Final Report

AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base, NM 87117

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This final report was prepared by the Experimental and Mathematical Physics Consultants, Santa Monica, California, under Contract F29601-75-C-0107, Job Order 46950323 with the Air Force Weapons Laboratory, Kirtland Air Force Base, New Mexico. Capt R. Gardner and Mr W. Bell (DYC) were the Project Officers-in-Charge.

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This report has been reviewed by the Office of Information (OI) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

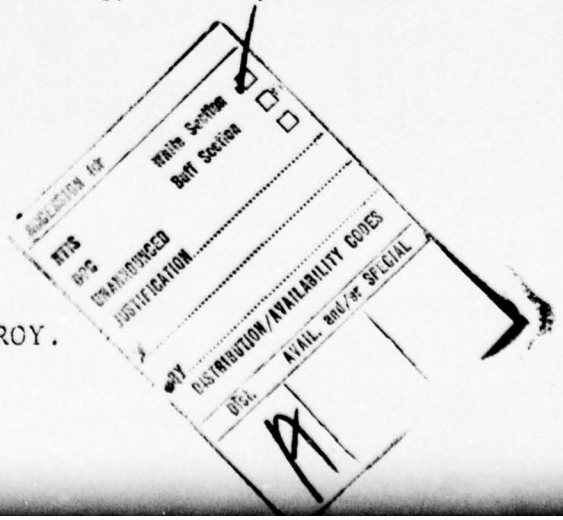
This technical report has been reviewed and is approved for publication.

William D Bell
WILLIAM D. BELL
Project Officer

FOR THE COMMANDER

M. T. BARNETT
Major, USAF
Ch, Satellite & C^3 Branch

PAUL J. DAILY
Colonel, USAF
Ch, Technology & Analysis Division



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The MASTER Program File is a collection of subprograms and data libraries used in solving radiation transport problems. This report describes methods and models used in the program. Program capabilities range from 1-dimensional problems through complex geometry, nonlinear, time-dependent problems. Particle physics models include primary and secondary photons, electrons, neutrons and heavy charged particles. Numerical methods include approximate transport kernels, direct numerical integration and MONTE CARLO quadratures.

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CONTENTS

SECTION I
INTRODUCTION

The MASTER program file contains programs and cross-section libraries used in solving radiation transport problems. This program file includes as subsets the FASTER, BETA, and TEMPER programs (refs. 1-8) and other analysis procedures which all operate from a common data base. The program is organized to take advantage of the similarities in different transport problems. This organization includes input processors which accept general descriptions of geometry, source distribution, detector distribution, and particle cross sections.

The program data base features variable format data input with variable dimension data storage. The input for data base preparation, and for invoking analysis procedures, are given in the Users Guide. This guide is maintained as an updatable card image file as part of the program file. Control cards for listing this guide, and for executing a problem, are summarized in the Appendix.

Analysis capabilities range from simple, one-dimensional problems through complex geometry, nonlinear, time-dependent problems. Particle physics models include primary and secondary photons, electrons, neutrons, and heavy charged particles. Numerical methods include approximate transport kernels, direct numerical integration, and Monte Carlo quadratures.

The general analysis procedures use Monte Carlo methods. For the more simple analyses, the Monte Carlo method can be understood in the context of particle simulation. These

general analysis procedures are implemented in the program structure by serial execution of three modules

a. Data base preparation; input and interpretation of data describing the transport problem (subprogram DEFINE)
b. Particle tracking; simulation of particle interactions while accumulating contributions to detector response using physics models appropriate to the analysis (subprogram SOLVIT)
c. Output; reduction and printout of sample statistics for the accumulated detector response (subprogram ANSWER)

Analysis procedures are described by starting with general models and then proceeding through specific models. The interplay of physics models is described first. This description is given relative to an electron-bremsstrahlung problem. Specific analysis methods are then described and their requirements relative to the data base established. Finally, methods and models implied by the data base are described.

Recommendations for simplifying program use, for minimizing system impact (reducing computer core and time requirements), and for improving physics models are given in the final section.

SECTION II
FUNDAMENTALS

The coordinates of particles are denoted by the phase space vector P which has the natural partitions

$$P = \underline{x}, \underline{u}, E, t \tag{1}$$

where $\underline{x}$ denotes position, $\underline{u}$ denotes direction, E denotes kinetic energy, and t denotes time.

A transport problem is described by;

a. The fixed differential source, $S^{O}(P)$

b. The fixed differential response, $D^{O}(Q)$

c. The microscopic total and differential cross sections for interaction and the spatial distribution of material mixtures

The distribution of material mixtures will be assumed constant over subsets of space, called regions, with discontinuous changes at region boundaries, called surfaces.

Macroscopic cross sections, both total and differential, are formed by number density weighting of the microscopic cross sections. This weighting procedure is implied in the following discussions where microscopic cross-section notation is used.

The effects of particle interactions are expressed in terms of cross sections as the no-interaction kernel (the differential flux per unit source)

$$N(P,Q) = \exp(-\sigma r)\ \delta_r(Q - U(P,r)) \tag{2}$$

where σr denotes optical thickness (mean-free-paths)

$$\sigma r = \int_0^r \sigma(U(P,r'))\ dr' \tag{3}$$

and the single-interaction kernel (the differential source per unit flux)

$$I(Q,P) = \frac{d\sigma}{dp}(Q,p)\ \delta_p(P - V(Q,p)) \tag{4}$$

In general, $\delta_t(...)$ is the Dirac delta function in all components of the argument except t. Thus, U(P,r) denotes the phase space coordinates of a particle which started at P and has traveled the distance r, and V(Q,p) denotes the phase space coordinates of a particle which enters an interaction with coordinates Q and whose phase space vector component q has been changed to p by the interaction.

It is sufficient to represent the solution of the transport equation by a Neumann series

$$\phi^k(Q) = \int S^k(P)\, N(P,Q)\, dP \tag{5}$$

$$S^{k+1}(P) = \int \phi^k(Q)\, I(Q,P)\, dQ \tag{6}$$

$$R^k = \int \phi^k(Q)\, D^0(Q)\, dQ \tag{7}$$

where $k = 0, 1, \ldots$ denotes the number of particle interactions, R^k denotes the integral response of the detector from exactly k interactions, and the iteration process is terminated when the response from all future interactions is deemed negligible.

The Monte Carlo method is used to evaluate the Neumann series integrals, i.e.

$$S^k = S^k(P_k) \,/\, p_k^*(P_k) \qquad P_k \in p_k^*(P) \tag{8}$$

$$\phi^k(Q) = S^k\, N(P_k,Q) \tag{9}$$

$$\phi^k = \phi^k(Q_k) \,/\, p_k^*(Q_k) \qquad Q_k \in p_k^*(Q) \tag{10}$$

$$S^{k+1}(P) = \phi^k\, I(Q_k,P) \tag{11}$$

The discrete phase space vectors P_k and Q_k are selected at random from the probability density functions $p_k^*(P)$ and $p_k^*(Q)$ which are defined such that

$$p_k^*(P) > 0 \quad \text{if} \quad S^k(P) > 0 \tag{12}$$

$$p_k^*(Q) > 0 \quad \text{if} \quad \phi^k(Q) > 0 \tag{13}$$

and normalized such that

$$1 = \int p_k^*(P)\, dP = \int p_k^*(Q)\, dQ \tag{14}$$

If the probability density functions are defined as

$$p_k^*(P) = S^k(P) \Big/ \int S^k(P)\, dP \tag{15}$$

$$p_k^*(Q) = \phi^k(Q) \Big/ \int \phi^k(Q)\, dQ \tag{16}$$

then the Monte Carlo integration reduces to a direct simulation of particle transport with nonabsorption and nonescape weighting.

Random Sampling

The random selection of discrete phase space vectors P_k and Q_k implies random selection of individual components of these vectors from marginal/conditional distributions. Random sampling techniques used for each phase space vector component all utilize random numbers, denoted by r, uniformly distributed on the open interval (0,1).

Solution of inverse functions is used for sampling simple continuous distributions

$$P^*(x) = \int_{-\infty}^{x} p^*(x')\, dx' = \int_0^r dr' = r \tag{17}$$

$$x = P^{*-1}(r) \tag{18}$$

For example, a point uniformly distributed on the open interval (a,b) is obtained as

$$\int_a^x \frac{dx'}{b-a} = \frac{x-a}{b-a} = r$$

$$x = a + r\,(b - a) \tag{19}$$

Table lookup of tabulated cumulative distribution functions is used for complicated distributions

$$\int_{-\infty}^{x} p^*(x')\,dx' = P_i^* + \frac{x - x_i}{x_{i+1} - x_i}\,(P_{i+1}^* - P_i^*) = r$$

$$x = x_i + \frac{x_{i+1} - x_i}{P_{i+1}^* - P_i^*}\,(r - P_i^*) \tag{20}$$

where x_i , $i = 1, 2, \ldots,$ are points at which the cumulative distribution is tabulated and the interval, i, containing the point x is determined as

$$P_i^* < r \leq P_{i+1}^*$$

$$P_i^* = \int_{-\infty}^{x_i} p^*(x')\,dx' \tag{21}$$

Rejection techniques are used to sample some analytic functions, e.g.

$$p^*(x) = \frac{g(x)\,h(x)}{C} \tag{22}$$

where

$$C = \int_{-\infty}^{\infty} g(x)\, h(x)\, dx$$

$$0 < h(x) \leq 1$$

$$1 = \int_{-\infty}^{\infty} g(x)\, dx$$

$$G(x) = \int_{-\infty}^{x} g(x')\, dx' \qquad (23)$$

The distribution is sampled as

$$x = G^{-1}(r) \quad \text{if } h(x) > r' \qquad (24)$$

where $G^{-1}(r)$ is the function inverse to $G(x)$ and r and r' are two different random numbers on (0,1). The procedure is repeated until an x satisfying the acceptance condition is selected. The normalizing constant C is the efficiency of the technique, i.e., the average number of repetitions to obtain an acceptable x.

Random sampling of summations is a particular interpretation of sampling continuous distributions, e.g., discrete interaction

events can be selected at random using

$$I(Q_k,P) = \sum_e I_e(Q_k,P) = \sum_e \frac{I_e(Q_k,P)}{p_k^*(e)} \; p_k^*(e)$$

$$= I_{e_k}(Q_k,P) \; / \; p_k^*(e_k) \qquad e_k \in p_k^*(e) \qquad (25)$$

where equality is in the expected (average) value sense, the subscript e denotes different events, and the probability density function has the properties

$$1 = \sum_e p_k^*(e)$$

$$p_k^*(e) > 0 \quad \text{if} \quad \int I_e(Q_k,P)\, dP > 0 \qquad (26)$$

The particular event e_k is selected using a random number r on (0,1) as

$$\sum_{e=1}^{e_k - 1} p_k^*(e) < r \leq \sum_{e=1}^{e_k} p_k^*(e) \qquad (27)$$

Sample Problem

To illustrate the Neumann series integration, a simple geometry is assumed. It will suffice to consider a semi-infinite plate containing a single material.

The description of the problem geometry requires the selection of a reference coordinate frame. For convenience, the material slab is oriented perpendicular to the z-axis with its bottom on the x-y plane such that its thickness is measured in the +z direction. Letting h denote the slab thickness, the material is bounded by two plane surfaces

$$z = 0$$

$$z = h$$

The position of particles within the material is denoted generally by $\underline{x}$ and, more specific, by the rectangular coordinates

$$\underline{x} = (x,y,z) = (x_1,x_2,x_3) = x\,\underline{i} + y\,\underline{j} + z\,\underline{k} \qquad (28)$$

Much more general problem geometries can be described. The concepts used in more general problems are discussed under the data base description.

A source of radiation is needed to make the problem meaningful. A monoenergetic electron beam is assumed to impinge on the bottom of the slab. For simplicity, the beam is assumed to have no breadth and to enter the material slab at the origin. Thus the coordinates of electrons, as they enter the slab, are

$$\underline{x}_0 = (0,0,0)$$

The initial direction of the electron beam is given by the polar angle ϕ measured from the z-axis, and the azimuthal angle θ measured from the x-axis. For the described problem, the initial azimuth is not critical. It will come into play as the particle traverses the slab.

It is convenient to denote directions by direction cosines relative to the three coordinate axes, i.e.,

$$\underline{u} = (\alpha,\beta,\gamma) = (c_1,c_2,c_3) = \alpha\,\underline{i} + \beta\,\underline{j} + \gamma\,\underline{k} \quad (29)$$

where

$$c_1 = \cos\theta \quad \sin\phi$$

$$c_2 = \sin\theta \quad \sin\phi$$

$$c_3 = \cos\phi \quad (30)$$

The cosine of the polar angle will almost always be used rather than the polar angle.

In a more general problem, the radiation source may have a spatial extent in one or more of the three rectangular coordinates, or, equivalently, in one or more of the three spatial variables in cylindrical or spherical geometry source volumes.

The radiation source may also start in various directions ranging from the monodirectional beam described here to isotropic and even complicated distributions in the two angular variables.

Assuming the electron beam for the sample problem is monoenergetic, the initial particle energy is denoted by E_0. Particle energies are measured in MeV and denote the kinetic energy only. This electron can be visualized as a single particle or it can be said to represent the entire beam, depending upon a preference for relative or absolute calculated output units. The number of electrons represented by this one particle is called the weight and is denoted by W or S^0.

For more complicated sources, a spectrum of energies may be present in the source. This spectrum can be described by a tabulated distribution and would be sampled to obtain a single mono energetic particle using a tabulated distribution sampling technique, i.e., table look-up.

Assuming the beam of particles enters the plate at a reference time t = 0, completes the specification of the initial phase space coordinates.

Electron Tracking

The first step in tracking a particle is determining the maximum distance, and the materials traversed, for the problem geometry. The simple slab geometry yields the general distance

$$s = (h - z_3) / c_3 \qquad \text{if } c_3 > 0$$

$$s = -z_3 / c_3 \qquad \text{if } c_3 < 0 \qquad (31)$$

The next step in particle tracking is determining whether the particle has an interaction within the defined geometry or leaks out through one of the boundaries of the problem geometry.

Electrons have a large number of interactions with the orbital electrons and with the field of the nucleus as they traverse material. It is computationally inefficient to treat each of these interactions explicitly. Instead, the electron is allowed to traverse a small distance ignoring interactions. At the end of the free flight, the electron coordinates are corrected for the net effect of the interactions ignored on the free flight. This procedure is called the condensed history method.

The first material effect on electrons (and other charged particles) is continuous energy loss along the free flight path. The processes causing the energy loss are inelastic interactions with the atomic electrons (with creation of secondary electrons) and radiative interactions with the field of the nucleus (with creation of bremsstrahlung photons).

The effect of these energy loss terms is denoted by L(E) and for electrons and other charged particles is called the stopping power. Stopping powers have units of MeV/cm and represent the average energy loss per unit distance traveled by the particle. There is an equivalent quantity for neutral particles which has the same definition but is usually called the linear energy transfer coefficient and, for photons, the energy absorption coefficient.

In a general sense, L(E) can be calculated as

$$L(E) = \int_0^E \frac{d\sigma}{dE'}(E,E')\ (E - E')\ dE' \tag{32}$$

where $d\sigma/dE'$ is the probability (cross section) per unit path length for scattering the particle from energy E to E', per unit scattered energy, and (E - E') is the energy lost in the scattering process. Written in this form there is an implied summation over different reactions for a given element of the material and, for multiple element materials, an atom density weighted summation over the elements.

The electron free-flight path length is determined using the stopping power. The path length is fixed by allowing the electron to lose a fraction, f, of its current energy which yields the implicit definition of the free-flight distance, d

$$d = \int_{E - f\,E}^{E} \frac{dE'}{L(E'(s'))} \tag{33}$$

After the electron traverses the distance d, particle coordinate updates are made

$$E_k = E - f\,E$$

$$\underline{x}_k = \underline{x}_{k-1} + d\,\underline{u}_k \tag{34}$$

where the index k denotes the number of electron steps since the history was started.

From the updated position, it can be determined if the particle escapes the material slab. If x_3 is less than zero, the electron has escaped from the incident side and is called a reflection. This cannot occur on the first step of course. If x_3 is greater than the slab thickness, the particle has escaped from the top of the slab and is said to be transmitted.

The time of the particle is also updated as

$$t_k = t_{k-1} + \int_0^d \frac{ds'}{v(E'(s'))} \tag{35}$$

where v(E') is the instantaneous particle speed (cm/sec)

$$v(E) = \frac{\sqrt{E\,(E + 2\,m_o c^2)}}{E + m_o c^2} \tag{36}$$

where c is the speed of light (not to be confused with any of the direction cosines), m_o is the particle rest mass, and $m_o c^2$ is the particle rest energy.

If the particle has not escaped from the material slab, the next procedure is to account for the interactions neglected on the free-flight path. These neglected interactions include the net effect of multiple angular deflections and the net effect of energy losses less than and greater than the mean loss.

The effect of the angular deflections is measured relative to the direction $\underline{u}_k$. The deflection is assumed equiprobable in azimuth around this fixed direction and varies with the cosine of a polar angle measured relative to this fixed direction as dictated by the Goudsmit-Saunderson distribution

$$p(\mu) = \sum_{n=0} A_n(d)\, P_n(\mu) \tag{37}$$

$$A_n(d) = \frac{2n+1}{2} \exp\left[-\int_0^d \sigma_n(s')\, ds'\right] \tag{38}$$

$$\sigma_n(s) = \int_{-1}^{1} \frac{d\sigma}{d\mu}(\mu) \left[1 - P_n(\mu)\right] d\mu \tag{39}$$

where $d\sigma/d\mu$ is the macroscopic angular deflection cross section (per unit deflection angle cosine) and $P_n(\mu)$ is the nth Legendre polynomial.

Since the angular deflection is sharply peaked in the forward direction, the multiple deflection distribution has a similar, but not as severe, forward peaked distribution. The cosine of the deflection polar angle, relative to $\underline{u}_k$, is obtained by random sampling of a cumulative distribution function tabulated on a fixed mesh of electron energies and deflection cosines.

With the random selection of an azimuth around $\underline{u}_k$, the direction cosines of the electron in a coordinate system with z-axis along $\underline{u}_k$ are denoted by (c'_1, c'_2, c'_3). These direction cosines are rotated to the reference coordinate system as

$$c_j = \sum_{i=1}^{3} c'_i \, R_{i,j} \qquad j = 1, 2, 3 \qquad (40)$$

where the rotation matrix R is determined by the polar and azimuthal angles of $\underline{u}_k$ measured in the reference system

$$R = \begin{bmatrix} \cos\theta_k \cos\phi_k & \sin\theta_k \cos\phi_k & -\sin\phi_k \\ -\sin\theta_k & \cos\theta_k & 0 \\ \cos\theta_k \sin\phi_k & \sin\theta_k \sin\phi_k & \cos\phi_k \end{bmatrix} \qquad (41)$$

The same rotation procedure is used on all particle reactions.

If bremsstrahlung photons are being created in the material slab, they can be modeled as created at random anywhere along the free-flight path or as created exactly at $\underline{x}_k$ with a slight error. The expected number of photons per electron created along the path is

$$\nu = \int_0^d \int_0^{E(s)} \frac{d\sigma}{dE_\gamma}(E(s), E_\gamma)\, dE_\gamma\, ds \qquad (42)$$

where $d\sigma/dE_\gamma$ is the macroscopic photon production cross section, i.e., the probability per unit path length and per unit photon energy of producing a photon with energy E_γ.

Several modeling possibilities arise. One is to use the expected number of photons produced and apply Poisson statistics to compute the actual number

$$p_n = \frac{\nu^n}{n!} \exp(-\nu) \qquad n = 0, 1, \ldots \qquad (43)$$

The actual value of n is obtained by random sampling this discrete density function. Each photon is given a weight equal to that of the electron and saved for later processing. At the same time, the electron energy can be decremented either for each photon so produced, or for the average energy of the produced photons.

If this electron energy decrementing procedure is used, the value of L(E) used in obtaining the free-flight path must exclude

the radiative stopping power. Otherwise the electron loses this radiative source energy twice.

An alternate procedure is to produce photons with weight equal to the expected production and use the total L(E) with no electron energy decrement during the electron transport.

Electrons can also excite the orbital electrons causing fluorescent photons. The expected number of excitations along the free-flight path is

$$n_i = \int_0^d \sigma_i(E(s))\, ds \qquad (44)$$

where $\sigma_i(E)$ is the cross section for exciting level i. Once excited, the atom produces fluorescence photons with probability Y_i where Y_i is the fractional fluorescence yield given excitation. Auger electrons and photoelectrons are also produced. All are saved for later processing.

The electron interaction modeling also includes the production of high energy secondary electrons. The expected number of secondary electrons produced with energies greater than Δ is computed as

$$n = \int_0^d \int_{E/2}^{E(s)-\Delta} \frac{d\sigma}{dE'}(E(s),E')\, dE'\, ds \qquad (45)$$

where $d\sigma/dE'$ is the macroscopic cross section per unit path length and per unit degraded energy for an electron to produce secondary electrons with energy E' and E" where E = E' + E". The cross section is given by Moller for electron-electron interactions. Two electrons always come out of this reaction. The electron with energy greater than E/2 is considered the primary and the electron with energy less than E/2 is called the secondary electron.

Given the expected number of high energy secondary electrons, there are several ways to proceed. The procedures are similar in logic to the creation of bremsstrahlung photons. One model uses Poisson statistics to determine the actual number of created secondaries. Another model creates one secondary electron with a relative weight equal to the expected number of secondaries. In both instances, the initial electron energy can be decremented by the actual or expected secondary energy. If the primary electron energy is decremented, then L(E) used to obtain the free-flight path must exclude those energy losses which correspond with the creation of secondary electrons.

The energy E' of any secondary electrons is determined by sampling the spectrum of secondary electron energies. This spectrum is simply the normalized Moller cross section which is stored as a tabulated cumulative distribution function on a fixed mesh of primary electron energies and of secondary electron energies (expressed as a fraction of the primary energy).

The direction of secondary electrons relative to the primary electron and the deflection of the primary due to secondary production are determined by the energy-angle relationship for electron-electron scattering.

The last model applied to primary electrons accounts for energy loss fluctuations. Here a Gaussian formula is used

$$p(E'' - E') = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-(E'' - E')^2 / 2\sigma^2 \right] \qquad (46)$$

where σ^2 is the mean-square deviation of the electron energy from the mean for the free-flight path and is computed as the path length integral

$$\sigma^2 = \int_0^d \int_0^{E(s)} \frac{d\sigma}{dE'}(E(s),E') \, (E - E')^2 \, dE' \, ds \qquad (47)$$

where $d\sigma/dE'$ is the differential energy loss cross section, i.e., the Moller electron-electron scattering cross section. The mean-square energy loss is stored as a tabulated table on a mesh of discrete energy points.

Energy loss fluctuations from radiative processes are modeled explicitly in the treatment of bremsstrahlung production. The secondary electron models which explicitly correct the primary electron energy for the produced secondary electron must exclude this energy loss range in the computation of the mean-square loss, i.e., the upper limit on the inner integration becomes $E(s) - \Delta$.

These same models are applied on each condensed history step of the electron until it escapes from the geometry or until the energy becomes so small that the electron residual range is much less than the dimensions of the material geometry. With small

residual energy, the flux spectrum as the particle goes to zero energy is determined from

$$\phi(E') = W\,E\,/\,L(E') \qquad 0 \leq E' \leq E \qquad (48)$$

During the electron tracking process numerous scores, based on the history of the particle, can be made. The obvious ones on a macroscopic scale are entrance, transmission, reflection, absorption, and energy deposited relative to the defined problem geometry.

From the definition that collision density equals flux times the total cross section, the flux in the slab can be estimated by dividing the particle weights going into collisions by the total cross section at their collision energy. For the condensed history technique, the implied total cross section is

$$\sigma(E) = L(E)/f\,E \qquad (49)$$

where f is the fractional energy loss per step. This same flux definition can be used to calculate scattered flux at an arbitrary point since the flux into collision times the differential scattering cross section yields the scattered source for all directions, in particular, the direction towards a detector point. Finally, the particle weight coming out of collision times the collision probability can be integrated along the path of potential collisions to yield the track length flux definition.

Photon Tracking

When the electron and any secondary electrons have been completely tracked, secondary photons are created and tracked. Two modes of photon creation were discussed during the electron tracking process. One mode is bremsstrahlung, which is forward peaked in angular distribution relative to the direction of the electron. The other mode is direct excitation fluorescence which is isotropic.

Since every electron path yields an expected number of both bremsstrahlung and direct excitation photons, both secondary production modes are considered. A decision is made at random at each photon production site (terminal points of the electron steps) to generate and track either the bremsstrahlung or the fluorescence photons. The decision is based on the total energy of the photons expected for the two modes and the initial weight of the photon is adjusted for this decision process.

Bremsstrahlung photons are created with an energy sampled from the normalized differential (per energy) production cross section. The direction, position, and time are set to the values of the primary electron at the step where the photon was produced.

This bremsstrahlung model assumes that the photons are produced in the same direction as the primary electron. Alternatively, the direction of bremsstrahlung photons relative to the electron is sampled from the double differential bremsstrahlung cross section normalized to form a probability density function. This requires an associated equiprobable azimuth selection and a rotation from the electron direction reference frame to the geometry reference frame.

Direct excitation photons are created with spectral weights based on the primary electron energy, weight, and step size

$$W_i = W\, d\, Y_i\, \sigma_i(E) \qquad i = 1, 2, \ldots \qquad (50)$$

i.e., a photon for each excited level. This spectrum is then sampled to obtain a single monoenergetic photon. The photon direction is isotropic and is sampled directly in the geometry reference frame.

Once created, the photon is tracked through the material slab until it leaks out, degrades below energy cutoff, or is absorbed.

The distance between photon collision points is calculated by one of several alternate methods. A simple particle analogy yields the distance (for a single material) of

$$d = \frac{1}{\sigma(E)} \ln(1 - r) \qquad (51)$$

If the distance d exceeds the distance to the boundary of the geometry, the photon has its collision in some part of the universe which was not modeled. By default, this collision is not germane to the problem. The photon escapes from the geometry and its history is terminated.

If the distance d implies a collision within the geometry, the next step involves the treatment of the interaction at the selected collision point. Before examining the interaction, it

is instructive to examine other methods for obtaining the distance between photon collisions.

In particular, the probability density function for collision points can be normalized to yield a collision point within the defined geometry

$$p^*(s) = \frac{\sigma(E)\ \exp(\ -\sigma(E)\ s\ )}{1\ -\ \exp(\ -\sigma(E)\ s_b\ )} \tag{52}$$

where s_b is the distance along the photon direction to the boundary of the material geometry. This probability density forces collisions within the defined geometry but requires a particle weight adjustment factor to compensate for the biased sampling

$$W' = W\ \frac{p(s)}{p^*(s)} = W\ (1\ -\ \exp(\ -\sigma(E)\ s_b\ )) \tag{53}$$

i.e., the particle weight is reduced by the nonescape probability.

Other collision density probability functions are often used. This is a relatively easy way to modify the physics of the sampled interactions to obtain those interactions deemed important to the transport problem. Particle weights are always adjusted to preserve expected values by multiplying by the ratio of the true probability density and the modified probability density.

The photon interaction event is selected at random by sampling the discrete probability density formed by the ratio of individual interaction cross sections to the total cross section. For some problems, this unbiased interaction selection is modified by an estimated importance of each interaction with a corresponding modification of the particle weight.

If Compton scattering is selected, the energy of the scattered photon is obtained by a rejection technique using

$$x = E/E'$$

$$g(x) = \frac{1}{\ln(1 + 2T)} \frac{1}{x} \qquad 1 \leq x \leq 1 + 2T$$

$$h(x) = x\,(x + 1/x - 1 + \mu^2)\,/\,2$$

$$\mu = 1 - (x - 1)/T$$

$$T = E\,/\,m_o c^2 \tag{54}$$

The direction and energy of both the photon and the recoil electron are determined by the mechanics of the Compton interaction.

If incoherent form factors are available, the photon and electron weights are multiplied by the bound electron correction factor, which is a function of element atomic number Z,

$$W' = W \quad S(q,Z) \; / \; Z \tag{55}$$

which is evaluated by linear interpolation of a tabulation versus q (momentum transferred)

$$q = \frac{E}{m_o c^2} \left(1 - 2\mu/x + 1/x^2 \right)^{\frac{1}{2}} \tag{56}$$

If photons are being tracked as polarized particles, a polarization vector $\underline{e}$ perpendicular to $\underline{u}$ is assumed (generated at random at the photon birth point). The decision to follow the polarized or unpolarized photon out of the interaction is based on the relative cross sections. If the perpendicular (random polarization after scattering) component is picked, an azimuthal angle is determined from the equiprobable azimuthal distribution. If the parallel mode is selected, the azimuthal angle is also sampled from the equiprobable distribution and the photon weight is adjusted to correct for this biased sampling.

If coherent scattering is the selected photon interaction, the cosine of the scattered angle is selected from the angular probability density function using a rejection technique

$$p(\mu) = 3\,(1 + \mu^2) / 8$$

$$g(\mu) = 1 / 2$$

$$h(\mu) = (1 + \mu^2) / 2 \qquad (57)$$

The weight of the photon is then reduced by the form factor

$$W' = W\,F^2(q,Z) / Z^2 \qquad (58)$$

which is tabulated versus momentum, q, transferred

$$q = \frac{E}{m_o c^2}\,(2\,(1 - \mu))^{\frac{1}{2}} \qquad (59)$$

If the photon was polarized, its azimuthal angle relative to the polarization vector $\underline{e}$ is left unchanged. If the photon is unpolarized, a random azimuthal angle is generated. The resulting $\underline{u}'$ direction relative to $\underline{u}$ is then rotated to the reference coordinate frame.

If pair production is the selected photon interaction, two annihilation photons are generated at the interaction site by increasing the photon weight by two, setting the energy to $m_o c^2$, and generating an isotropic direction.

This pair procedure is modified if pulse height distributions are being obtained, since it is necessary to track each of the annihilation photons separately.

The positron/electron pair are created by sampling an equiprobable energy distribution on $(0, E - 2m_o c^2)$. Both members of the pair are tracked as electrons. Their direction is selected from an exponential distribution which preserves the mean production direction.

If the photoelectric event is the selected interaction, the subshell of the interaction is determined proportional to the partial cross section $\sigma_i(E)$. The photon weight is multiplied by the fluorescence yield and the photon energy is set to the fluorescence energy. The corresponding direction is isotropic and is selected at random in the reference coordinate frame.

The Auger electrons associated with the photoelectric event are given isotropic directions. The photo electron direction relative to the photon direction is sampled using the rejection technique

$$g(\mu) = \frac{\eta^2 - 1}{2} \frac{1}{(\eta - \mu)^2}$$

$$h(\mu) = (\eta^2 - 1)(1 - \mu^2) / (\eta - \mu)^2$$

$$\eta = m_o c^2 / (E (E + 2 m_o c^2))^{\frac{1}{2}} \qquad (60)$$

The weight of the photo electron is multiplied by the factor $p(\mu) / p^*(\mu)$ where $p(\mu)$ is the Sauter or Fischer angular distribution and

$$p^*(\mu) = g(\mu)\, h(\mu) / C$$

$$= \frac{8}{3} (\eta^2 - 1)^2 \frac{(1 - \mu^2)}{(\eta - \mu)^4} \qquad (61)$$

The photon tracking continues by collision using similar logic on each collision until the photon escapes, its energy goes below a cutoff, or its weight becomes small.

During the photon tracking, scoring comparable to that for the primary electrons is performed.

SECTION III

ANALYSIS PROCEDURES

The MASTER program file contains several particle tracking procedures. Most of these procedures utilize part or all of the geometry, source, and detector data base implied in the previous section and discussed in more detail in the next section.

BETA-II Procedure (refs. 5 and 6)

BETA performs Monte Carlo electron-bremsstrahlung or photon electron transport by the methods outlined in Section II, predominantly analog Monte Carlo.

BETA uses the complete data base. Particle tracking is controlled by subprogram SOBER and includes an optional ability of treating the effect of fixed electric and magnetic fields. The fixed electric field option includes the nonlinear buildup of electric fields assuming frozen charge. This charge buildup is limited to two-dimensional cylindrical geometries. The solution of Poisson's equation for a fixed charge density is performed by subprogram VOLTS in the output module of the program.

For problems not requiring field effects, the BEAMAP procedure is recommended for its superior particle processing speed.

BEAMAP Procedure

BEAMAP is a faster version of BETA where no field effects are allowed (except for an electron reflection boundary) and all of the appropriate particle physics are collected into a single subprogram.

TEMPER Procedure (refs. 7 and 8)

TEMPER calculates time-dependent charge and current densities, scalar and vector potentials, and electric and magnetic fields in three-dimensional cavity geometries. A problem is initiated from a specified electron emission distribution. The time evolution of a problem is obtained by a series of time steps in which potentials are assumed constant. During each time step, typical electrons are sampled from the electron emission distributions and added to the electron population which existed at the end of the previous time step. Electrons are moved using relativistic kinematics which include Lorentz force, slowing down from gas in the cavity, and production of primary ionization electrons. At the end of a time step, a snapshot is taken of the time-averaged charge and current densities during that step. At the end of each time step, the scalar and vector potentials are calculated by performing volume integrations over the charge and current densities. Retarded time effects are explicitly calculated.

DIODE Procedure

This analysis procedure calculates quasi-static nonlinear electron transport between parallel plates. Electron emission is allowed from both plates. The energy dependence of emission is represented within a fixed group structure where each group can be subdivided for better representation of highly charge limited problems.

The angular dependence of emission must be an integral power of the cosine of the emission angle relative to the cavity surface normal. This angular dependence is represented by a

set of discrete intervals which preserve the total emission and the average emission angle.

Time dependence of the emission is either triangular or Poisson. The time dependent behavior of the cavity is determined by solving a series of quasi-static problems at successive points in time.

The cavity length is subdivided into intervals for representation of the spatial behavior of the electric field and of the electron transport between the plates. At each time step typical electrons are started from each emission surface and in every energy interval and direction interval. The contribution from these typical electrons to the charge density, current density, and cavity gas ionization are computed. The charge density and the net current density, in conjunction with a fixed impedence between the plates, are used to obtain the potential and electric field.

EMP3D Procedure

This analysis procedure calculates nonlinear electron transport in regular three dimensional geometries. A finite difference particle-in-cell approach is used.

Particle populations are represented by a fixed mesh in space, energy, and direction. Emission distributions have the same characteristics and can be defined at any mesh point.

SOBER Procedure (refs. 9-11)

This analysis procedure calculates neutron/photon transport using Monte Carlo methods. Extensive importance sampling is used.

SOBER uses the complete data base to obtain volume and surface averaged fluxes. Fluxes are also obtained at multiple point detectors. In general, this procedure is not used for point detectors in source and scattering volumes where explicit representation of point-to-point singularities are required. The FASTER analysis procedure is used for these point detector problems.

FASTER Procedure (refs. 1-3)

FASTER is used to obtain flux-at-a-point when the point is in a source or scattering volume. Monte Carlo methods are used to obtain both neutron or photon fluxes.

This procedure uses importance sampling which includes the point source and point detector singularities. Therefore, finite variance fluxes are always obtained.

The complete data base is used by FASTER including options for transport in helical ducts (ref. 12) and shield weight optimization (ref. 13).

PULSE, TRICK, TREAT Procedures (refs. 14 and 15)

PULSE performs parametric electron transport calculations of charge and energy deposition, reflection, transmission, and pulse height distributions. The procedure combines Monte Carlo and numerical integration procedures. An electron track is initiated at the maximum energy of interest and followed through an infinite medium by Monte Carlo methods. The track at various degraded energies is used to characterize electron sources at these lower energies. The track, or any residual part used for lower energies, is then rotated and translated numerically to yield information for various initial directions and material thicknesses. The procedure is repeated for multiple tracks to converge the Monte Carlo aspect.

TRICK and TREAT calculate pulse height distributions for small volume detectors inside complicated geometries by numerical integration using either approximate transport kernels (TRICK) or interpolations of tabulated Monte Carlo transport data (TREAT). Both primary and secondary radiations contribute to the pulse heights. Major allowed primary sources are neutrons producing activation, photons, and electrons.

ANALOG Procedure

This analysis procedure uses analog Monte Carlo techniques to simulate photon interactions within a complex geometry pulse height detector system. The detector is assumed to reside within a laboratory mockup. Importance sampling is used to increase the number of particles which enter the detector both directly or by scattering from the facility structure.

SHIELD and SIGMA Procedures (refs. 16 and 17)

SHIELD numerically integrates the electron-bremsstrahlung transport equation for one dimensional geometries to obtain dose and other flux responses versus shield thickness. Cross section data and response functions are obtained from the data base.

SIGMA calculates space radiation dose at points in complicated geometries by a solid angle integration about the point using interpolated one-dimensional dose transmission kernels, e.g. SHIELD results. SIGMA uses the geometry and detector portions of the data base.

ADJOINT Procedure (refs. 18 and 19)

This Monte Carlo procedure performs electron and photon transport calculations by tracking particles backward from the detector to the source. It is used for point or small detector calculations in extended source fields, e.g., space radiation sources. Capabilities include dose calculations, pulse height distributions, and parametric dose attenuation data for electron sources and secondary electron flux/dose for primary photon sources. The complete data base is used.

SECTION IV

DATA BASE

The data base is shared between subprograms through named common blocks and blank common. The layout of these areas is

a. Blank common contains data arrays. Each data array has variable dimensions and arrays are packed into ascending locations according to the current array dimensions.
b. Named common blocks contain fixed location data. In particular, the addresses and dimensions of data arrays are stored in named common blocks.

These areas are initialized before processing user data by subprograms BOOTIT, which initializes executive data arrays, DATBAS, which allocates arrays used for problem description, and DATRUN, which allocates arrays used during the problem solution.

Input, preparation, storage, and use of the data base is divided into many procedures. This division simplifies the description and modification of transport problems. Each procedure is controlled by user directives. These procedures are described under the general categories

a. Executive procedures
b. Geometry
c. Source
d. Detector
e. Physics

Executive Procedures

All procedures are controlled by user supplied data. Each procedure involves a block of consecutive data cards. The first card of the block is the "header card" and contains the name of the procedure, where the first three letters are unique, e.g., STOp. The second card of the block is the "limit/option card" and specifies, as integer data, array limits and options for the designated procedure.

When a procedure is recognized, the limits and options are stored in appropriate locations of the named common blocks. Array storage is reallocated (subprogram IARRAY) if any array dimensions have changed. If the procedure requires local data arrays, these arrays are allocated to blank common at the end of the data base arrays using subprogram INDEX. This local data storage area is recovered after the procedure is completed.

Input data required by a procedure is processed by subprogram READER. During the input process, the following options are available

a. Fixed or variable format data with variable format data separated by blanks or commas
b. Repeat and interpolation of data elements. Interpolations include exponential, logarithmic, linear and power laws 2 through 9
c. Conversion of specified data elements, e.g., degrees to radians, exponentiation, and other function evaluations

Arguments passed to the data card processor indicate whether the input data has specific units and order. This information permits data conversion to standard units during the input process. It also allows checking arrays for order consistency. Other errors detected during the input process include data out of range, indices out of range, and missing data.

Obvious executive procedures are the call, by name, of the analysis procedures, e.g., BEAmap. For analysis procedures, the limit/option card contains the number of histories and other integers which control the particle tracking. When an analysis procedure is recognized, the following operations are performed

a. Missing data is noted and where possible supplied by the program
b. The dimensions of data arrays used for particle tracking are set to necessary values for problem solution
c. If the problem setup has no detected errors, the analysis is performed. If errors were detected, the analysis step is aborted.

A problem is terminated by the STOp procedure. An optional formatted dump of the data base is obtained prior to the programmed stop. This data base dump includes each named common block and each variable dimension array.

A dump of the entire data base, or of specified named commons and arrays, can also be obtained at the entrance and exit points of major subprograms. The necessary control information is supplied as data using the DUMp procedure.

Long running problems can be solved using multiple runs. A restart file is specified using the TAPes procedure. The information written on the restart file is retrieved in a subsequent computer run using the CONtinue procedure. The analysis is continued using the history counter, accumulated scoring, etc. contained on the restart file.

Trivial executive procedures include

a. LABel, for entering printout headings
b. NEXt, to increment the problem identification number
c. ZERout, to re-initialize between independent problems
d. RANdom, to override the default random number

Some executive procedures alter, in some manner, the processing of data by the problem related processors

a. PRInt, suppresses the printout of extensive input cards
b. UNIts, indicates that some inputs have nonstandard physical units, e.g., energies in keV, geometry dimensions in feet, etc.
c. ADDress, supplies index modifiers for problem data input by index, e.g. geometry, sources, and detectors. This procedure simplifies the collation of two independent problems into a single problem.

Finally, data can be directed to the data base using

a. BLOck, specifies the value of elements of named common blocks
b. ARRay, accepts variable dimension arrays by name

Geometry

The transport problem geometry is described by disjoint volumes called "regions" where the boundaries of regions are called "surfaces". Each region has constant material properties denoted by a composition or material identifier and a density relative to the reference density of that material.

The problem geometry can be compact, i.e., containing no undefined volumes, or contain undefined volumes. All undefined volumes are assumed to be void. In particular, the space surrounding a compact geometry is assumed to be void. A compact geometry implies that the surface forming the boundary between adjacent regions is unique.

Geometry related calculations assume that all surfaces are described by the quadric equation

$$\begin{aligned} U(\underline{x}) = {} & a_0 + a_1 x + a_2 y + a_3 z \\ & + a_4 x^2 + a_5 y^2 + a_6 z^2 \\ & + a_7 xy + a_8 yz + a_9 zx \end{aligned} \tag{62}$$

where a_i , $i = 0, 1, \ldots, 9$, are constants. $U(\underline{x})$ is zero for points on the surface, $U(\underline{x})$ is less than zero for points "inside" the surface, and $U(\underline{x})$ is greater than zero for points "outside" the surface. The inside/outside sense can be reversed by multiplying the surface equation by -1.

Description of a geometry using these quadric surfaces is tedious. Therefore, a number of processors are used to simplify the description task. These processors, as a group, are contained in subprogram GEOMIN.

Geometry related calculations include

a. Determining the region occupied by a point, performed by subprogram LOCATE
b. Ray tracing from a point in a fixed direction to determine the order and thickness of materials encountered along a particle path, performed by PATH
c. Calculating the surface normal at specific boundary crossings, performed by subprogram NORMAL

The numerical operations performed during these calculations are detailed in references 1, 5, and 20.

Some transport problems have simple geometries. It is sufficient for these problems to describe the material geometry using one of the following processors

a. SPHere, for concentric spherical zones. For the particular problem of transport in an approximation of a spherical exponential atmosphere, the AIR processor supplies the density versus altitude variation.
b. CYLinder, for cylindrical geometries with azimuthal symmetry
c. SIMple, for regular meshing of the three orthogonal coordinates of rectangular, cylindrical, or spherical geometries

These procedures assume a single material in all regions. This assumption is countermanded using the ARRay processor for the specific array MTL which contains the material identifier.

More complicated geometries often use direct description of surfaces and regions. These descriptions can be used to augment a subset of the geometry described by the more simple geometries, or these descriptions can be used to specify the entire geometry.

Direct surface description is accomplished with the SURface processor. This processor accepts the coefficients for the general quadric surface. Alternatively, simple surfaces are recognized in more simple forms and expanded by the processor to the quadric form. These simple forms include

a. Planes perpendicular to one of the coordinate axes
b. Planes parallel to one of the coordinate axes
c. Cones parallel to a coordinate axis
d. Cylinders and elliptic cylinders parallel to an axis
e. Spheres and ellipsoids

Some regions have helicoid or torroidal boundaries. The corresponding surface equations are specified with the HELix processor. These surface equations utilize a special intersection calculation during ray tracing (ref. 21).

Direct region description is performed via the REGion processor. The description includes

a. Material identifier and relative density
b. Boundary surface list
c. Coordinates of any point in the region

The point-in-region coordinates are used to determine the inside/outside sense of the region relative to the boundary surfaces.

A SURface and REGion description of problem geometries can also get tedious. This has led to the following processors, which have a limited applicability

a. BOArds, for describing parallel material slabs with different compositions and common transverse boundaries
b. BOXes, for describing multiple layer boxes, cylinders, and spheres embedded in regions
c. BAYs, for describing the exterior skin and interfaces between multiple bay spacecraft
d. DIVide, for subdividing regions into smaller components

A more general procedure for simple description of regular geometry regions is DESign. This procedure combines the surface and region description for the following shapes

a. plates
b. elliptical cylinders
c. spheres and ellipsoids
d. cylindrical annuli
e. truncated cones

This procedure shortens the geometry description but requires extreme care in data preparation so that surfaces forming a common boundary between two regions are recognized, i.e., dimensions supplied with exactly the same significant digits. The procedure assists in this recognition by checking for volumetric overlap of the regions.

Some geometries involve regular surfaces not aligned with the coordinate axes. The description of these surfaces is accomodated directly with the SURface processor. The description is simplified, however, by using the ROTate processor.

The ROTate processor operates on specified surfaces and regions. Operations include rotations or translations, any number and in any order. The same processor can be applied to the geometry of fixed sources and detectors.

The description of some problem geometries is simplified by invoking the SYMmetry processor to delineate the surfaces of symmetry. However, this procedure cannot be used for analysis procedures which perform flux-at-a-point calculations.

Verification of a geometry description includes several self-consistency checks performed by subprogram REGION. The most useful checking is provided by exercising the ray tracing operations during the generation of geometry pictures using the PICture processor for printout display and the CAMera processor for cathode ray tube (CRT) display. Both processors require specification of the geometry frame to be viewed. Both will also project the trajectories of particles generated during short runs of the Monte Carlo analysis procedures.

Source

The fixed radiation source can be supplied with a generality commensurate with that of the problem geometry. Single or multiple sources can be defined using the SOUrce processor. The description of each source includes the spatial, angular, and energy distribution of emitted particles. Time dependence is not required for many problems and is discussed as a separable topic.

The geometric characteristics of each source are specified by the following information

a. source geometry, rectangular, cylindrical, or spherical
b. separable tabulated distribution functions for each of the three spatial variables
c. a translation vector

Irregular shaped sources can be specified by rejecting regular geometry source points which are outside specific geometric regions.

The tabulated spatial distributions can be a discrete point (a delta function) or multiple points. This flexibility yields point, line, surface, or volume distributed sources. The distribution functions are accepted as unnormalized relative density functions.

The angular character of a source is specified by a tabulated distribution in each of the two angular variables. The tabulated distribution is an unnormalized relative density function with a single point (delta function) or multiple points. This yields monodirection or angularly distributed, including isotropic,

sources, depending upon the number of points in each distribution. The interrelationships of the spatial and angular variables is discussed in the Users Guide. The numerical techniques for normalizing and interpolating the tabulated distributions are given in references 1 and 5.

Many options are provided for describing the particle energy spectrum including

a. Tabulated differential number spectrum
b. Tabulated differential intensity spectrum
c. Tabulated interval number or intensity spectrum
d. Tabulated integral number or intensity spectrum
e. Analytic functions for fission neutrons, black bodies, fission gammas, Gaussian, Poisson, and self-rectified electron beam

The fixed source is normalized to a specified total yield in particles or energy. Alternatively, the input source can be arbitrarily scaled or forced to match a specified density at a particular point.

Time dependent problems with nonlinear aspects require that a time profile be supplied using the PROfile processor. For linear problems, this time profile is used in a convolution of time dependent response, i.e., in linear problems all particles are born at t = 0. Extremely short time analyses of nonlinear problems require the WAVefront processor to specify the time of arrival of the radiation wavefront.

In the absence of importance sampling, particles are sampled from the fixed source in an analog fashion. The analog sampling can be modified in several ways. Stratification by source, spatial interval, and angular interval can be selected through the option card for the analysis procedure. The relative frequency of sampling particles from each source can be modified through the RELative processor. The frequency distribution for each of the spatial and angular source variables can be modified using the RATio processor. Finally, for volume distributed sources and point detectors, the $1/r^2$ and exponential fall off of source importance with separation distance can be included by the PSEudo source processor.

Detector

The description of detectors has a similarity to the description of sources. However, detectors are assumed to have the same sensitivity for all positions and directions in their sensitive volume.

Macroscopic information on particle transport is obtained with the DEPosition and LEAkage processors. These processors yield information on the total number and energy statistics and no information on variation with particle energy. For problems with extensive importance sampling, e.g., flux-at-a-point simulation, the resulting output may have little, if any, usefulness.

Similar, but more definitive detector information is obtained from the CHAnnel processor. Here the deposition in specified

geometric regions is partitioned into multichannel output of deposition or energy loss per particle. This pulse height information can be convoluted with a specified smearing distribution using the NOIse processor.

More detailed transport results are obtained for detectors described using the DETector processor. These detectors can consist of points, geometry regions, and boundaries of geometry regions. Results for several detectors can be added using the SAMe detector processor.

Angular information for these specific detectors can be obtained using the ANGular processor which yields Legendre moments of the angular flux, in particular the forward and backward current. These moments are reconstructed to yield the azimuthally averaged angular flux distribution. Angular flux information can also be obtained from the SOLid angle processor for specified solid angle intervals.

Energy information for the specific detectors is given in the energy mesh used to tabulate cross sections. The FLUx processor can be used to establish a different output structure. The RESponse processor provides for weighting the energy dependent fluxes with either user specified response functions or response functions based on cross section information, e.g., energy absorbtion coefficients.

Time dependence for specific detectors is made relative to the minimum time of arrival using the TRAnslate processor. The time dependence is obtained by time interval using the TIMe processor and by an analytic moments, with reconstruction, method using the MOMents processor. Both of these time dependent outputs is convoluted with any source time PROfiles.

Sensitivity of the detector output can be obtained for source GROups, BIRth sources, BOUndaries crossed, ORDer of scattering, and SCAttering regions by using the indicated processor.

More detailed sensitivities can be obtained using the CORrelated processor. The correlation is on any combination of source and region material. A correlation for electron transport problems can be made only for the void/nonvoid configurations.

The FASTER flux-at-a-point analysis procedure can determine the variation in flux levels with respect to changes in region dimensions by using the NORmal processor to request derivative information, and the THIckness processor to specify incremental material thicknesses. The derivative information can also be used to determine a weight optimized shield configuration using the MINimum processor (ref. 13).

Importance sampling relative to detector response can be requested using the PREferred processor to specify a region where particle interaction densities should be increased. Conversely, the SHOrt circuit processor can be used to circumvent many of the default importance sampling models. The OPTimum processor can be used to request estimates of better importance sampling parameters based on variance partial derivatives.

Many of the detector outputs can be print plot displayed through the QUIck plot processor. The PLOt processor will display the differential flux spectrum if a drum plotter is available.

Particle Physics

Particle physics data consists predominantly of processed cross sections obtained from detailed data libraries.

The MATerials processor supplies partial densities of elements or isotopes in materials or compounds. The MIXture processor can be used for neutral particle problems to specify materials in which only the hydrogen content varies.

Non linear problems require the DIElectric processor to specify macroscopic electromagnetic properties. The CURrent processor is used to define initial fixed fields for the BETA analysis procedure.

Importance sampling of the particle physics is optional and includes BIAsing to set models for selecting particle collision points and scattered directions, CAPture to force an analog simulation of neutron slowing down, SKIn to artificially increase photon interactions near an electron emission surface, and SPAtial to increase or decrease collision densities in material regions.

The PHOton processor prepares photon cross-section data. Card input is accepted. However, the usual source of data is ENDF/B files 23 and 27 (ref. 22).

The ELEctron processor prepares electron cross-section data. Default models are those of the BETA and BETA-II programs described in references 5 and 6. Electron bremsstrahlung production models from references 23 and 24 are used. Alternatively, numerical data from reference 25 can be used for energies below 0.5 MeV. Direct excitation cross-sections are calculated by

the formalism of reference 26 but with explicit evaluation of subshell cross-sections from ENDF/B file 23.

The ELEctron processor will also accept electron/bremsstrahlung cross-section data from DATAPAC (refs. 27 and 28). This data is superior to the default data except for the photon transport and direct excitation cross-sections. These portions of the default data are used in preference to the corresponding portions of the DATAPAC library.

Heavy charged particle cross-sections are also developed by the ELEctron processor by selecting a corresponding option on the limit/option card.

Neutron and secondary gamma ray production data are obtained from ENDF/B data files (ref. 29) using the NEUtron processor. Alternatively, neutrons are simulated in the multigroup approximation using the MULtigroup processor and standard multigroup libraries (ref. 30). The multigroup libraries usually include coupled photon transport data. The secondary photon production data are stripped from these libraries using the SECondary procedure, and the photon transport data are discarded since the point value ENDF/B data are preferred.

SECTION V

RECOMMENDATIONS

The generality of the MASTER program file makes it difficult for novice users to select options and provide data for a problem. The following program modifications are recommended to eliminate the difficulty

a. Provide complete problem descriptions as defaults for each analysis procedure
b. Allow user override of the default data by keywords

For example, if a user wants to solve the default electron-bremsstrahlung transport problem, the input data for the default problem could consist of

```
,BEAMAP,ELECTRON,PHOTON/ Default Problem Execution
```

where the default problem parameters describe a tungsten target, plane-parallel monoenergetic source of 1 MeV electrons normal to the target, and a detector measuring backward and forward photon emission.

To change default parameters, keyword parameters could include

```
,BEAMAP,ELECTRON,PHOTON
,TARGET=GOLD
,SOURCE.DIRECTION=30DEGREES
,SOURCE.ENERGY=100KEV/
```

Similar default problems and keyword parameters would be available for each analysis processor.

For more complicated problem descriptions it is recommended that

a. Materials contained in geometric volumes be specified by name and density
b. Material compositions and standard densities be obtained from a library that contains all elements and the more common mixtures, alloys, and compounds
c. All macroscopic particle physics data be generated without intervention by the user

The program changes that accomodate these features would reduce a users task to describing the geometry, source, and detector of the problem.

The development history of the program file has required "patching in" of some physics models with a degradation in efficiency. The following program modifications are recommended to improve efficiency

a. Particle tracking be performed in a batch mode, i.e., perform the same operation on a series of histories before proceeding to the next operation
b. Precalculate as tables all primary to secondary transition probabilities

These modifications will also yield more efficient calculations on vector arithmetic computers.

APPENDIX

CONTROL CARDS

The users guide is obtained as a formatted listing using the following control cards on the Air Force Weapons Laboratory CDC 7600

```
TMJAA,T17,STMFZ.
ACCOUNT(NAME,NUMBER,GROUP,EXTENSION)
ATTACH(GUIDE,ID=DYSXTMJ)
COPYSBF(GUIDE,OUTPUT)
```

A problem is executed from the following control cards

```
TMJBB,T400,STMFZ.
ACCOUNT(NAME,NUMBER,GROUP,EXTENSION)
STAGE(MASTER,NT,HD,PRE,VSN=GL97,ST=ANY)
COPYP(MASTER,OLDGO)
COPYF(MASTER,TAPE9)
RETURN(MASTER)
REWIND(TAPE9)
LDSET(MAP=0,FILES=TAPE9)
OLDGO(PL=100000)
```

7_{8_9} end of record

problem data

$6_{7_{8_9}}$ end of file

REFERENCES

1. Jordan, T. M., FASTER, A Fortran Analytic Solution of the Transport Equation by Random Sampling, WANL-PR-(LL)-010, Westinghouse Astronuclear Laboratory, Pittsburg, PA, June 1967.

2. Capo, M. A. and T. M. Jordan, Sample Nuclear Rocket Reactor Problem for the FASTER Code, WANL-PR-(LL)-014, December 1967.

3. Jordan, T. M., FASTER-II, A Time Dependent, Generalized Geometry Monte Carlo Computer Program for the Transport of Neutrons and Photons, ART-41, A. R. T. Research Corporation, Los Angeles, CA, June 1970.

4. Jordan, T. M., FASTER-II(Revised), A Time Dependent, Generalized Geometry Monte Carlo Computer Program for the Transport of Neutrons and Photons, ART-56, July 1971.

5. Jordan, T. M., BETA, A Monte Carlo Computer Program for Bremsstrahlung and Electron Transport Analysis, AFWL-TR-68-111, Air Force Weapons Laboratory, Kirtland Air Force Base, NM, October 1968.

6. Jordan, T. M., BETA-II, A Time Dependent Generalized Geometry Monte Carlo Program for Bremsstrahlung and Electron Transport Analysis, ART-60, October 1971.

7. Jordan, T. M., TEMPER, A Computer Program for the Transport in Electromagnetic Fields of Photon and Electron Radiation by Monte Carlo and Finite Difference Techniques, ART-33, July 1969.

8. Jordan, T. M., The TEMPER Program, ART-64, March 1972.

9. Jordan, T. M., Reactor Shielding Calculations by the Monte Carlo Method, Douglas Paper No. 3271, Douglas Aircraft Company, Santa Monica, CA, May 1965.

10. Jordan, T. M., Energy-Independent Biasing Functions for Monte Carlo Transport Calculations, Douglas Paper No. 3636, November 1965.

11. Jordan, T. M., SOBER, A Monte Carlo Program for Neutron and Gamma Ray Transport in Complex Geometries, Douglas Report DAC-60659, May 1967.

12. Jordan, T. M. and M. L. Wohl, Neutron Streaming in Helical Ducts, NASA TM X-52725, NASA, Lewis Research Center, Cleveland, Ohio, December 1969.

13. Jordan, T. M. and M. L. Wohl, Shield Weight Optimization Using Monte Carlo Transport Calculations, NASA TM X-52973, March 1971.

14. Sensor/POST Analytical Model User's Manual, MDC G5036, McDonnell Douglas Astronautics Company, Huntington Beach, CA, April 1974.

15. Jordan, T. M., TRICK Numerical Models, EMP.L76.052, Experimental and Mathematical Physics Consultants, Los Angeles, CA, April 1976.

16. Jordan, T. M., SIGMA, A Computer Program for Space Radiation Dose Analysis Within Complex Configurations, Douglas Report DAC-60878, November 1967.

17. Davis, H. S. and T. M. Jordan, Improved Space Radiation Shielding Methods, TM 33-765, Jet Propulsion Laboratory, Pasadena, CA, March 1976.

18. Jordan, T. M., An Adjoint Charged Particle Transport Method, EMP.L76.071, July 1976.

19. Jordan, T. M., A Coupled Forward/Adjoint Monte Carlo Method, EMP.L76.072, July 1976.

20. Jordan, T. M., QUAD, A Computer Subroutine for Ray Tracing in Quadric Surface Geometries, Douglas Report SM-46333, December 1964.

21. Jordan, T. M., Helical Geometry Routine for the FASTER Computer Program, ART-25, January 1969.

22. Data Library DLC-7, Radiation Shielding Information Center, Oak Ridge National Laboratory, Oak Ridge, TN.

23. Koch, H. W. and J. W. Motz, "Bremsstrahlung Cross Sections", Rev. Mod. Phys., 31, pp. 920-955, 1959.

24. Pages, L. et al., Atomic Data, Vol. 4, No. 1, Academic Press, March 1972.

25. Lee, C. M. et al., "Electron Bremsstrahlung Spectrum, 1 - 500 keV", Physical Review A, 13(5), pp 1714-1727, May 1976.

26. Kolbenstvedt, H., "Simple Theory for K-Ionization by Relativistic Electrons," Journal of Applied Physics, 38(12), pp 4785-4787, November 1967.

27. Mack, J., Personal Communication on DATAPAC Compatibility, Los Alamos Scientific Laboratory, Los Alamos, NM, 1976.

28. Berger, M. J. and S. M. Seltzer, Electron and Photon Transport Programs, NBS Report 9836, National Bureau of Standards, Washington, D. C., June 1968.

29. Ozer, O. and D. Garber, ENDF/B Summary Documentation, ENDF-201 (BNL-17541), Brookhaven National Laboratory, Upton, Long Island, NY, May 1973.

30. DLC-31 Library, Radiation Shielding Information Center.